MANUAL

vs 3/95

NMR Database of Lignin and Cell Wall Model Compounds

by

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a collaboration between the
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USDA-Agricultural Research Service
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Introduction to NMR Database

This NMR database has been designed to aid plant cell wall chemists in general and lignin chemists in particular. By compiling data from a series of model compounds run under strict acquisition conditions in three solvents, we hope to provide a compilation useful for NMR research. Additionally, the database contains a selection (to be expanded) of literature data.

This Database is a collaborative effort between the US Dairy Forage Research Center and the US Forest Products Laboratory. The primary contacts and collaborators are:

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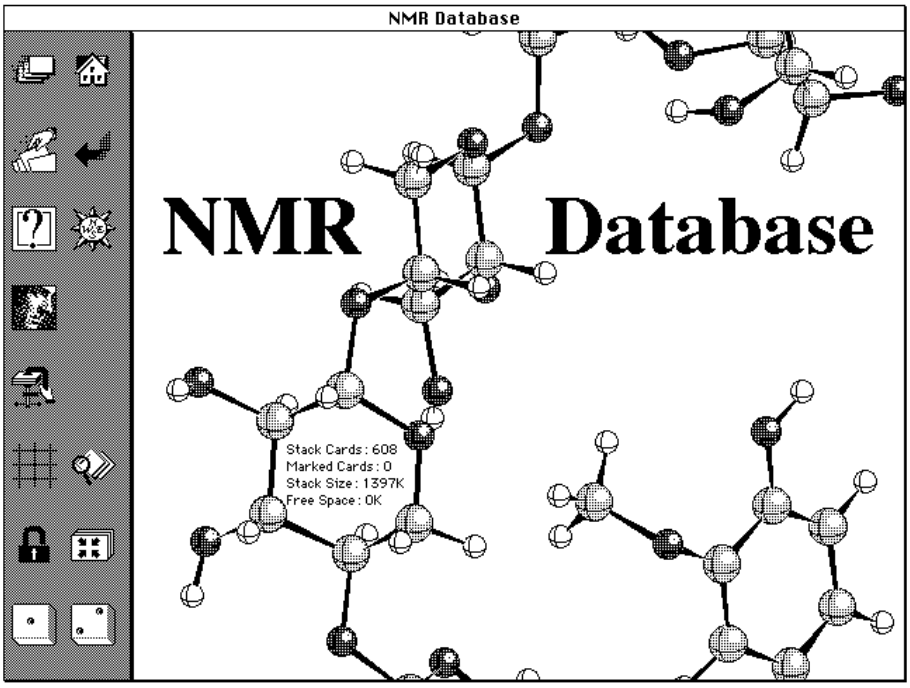
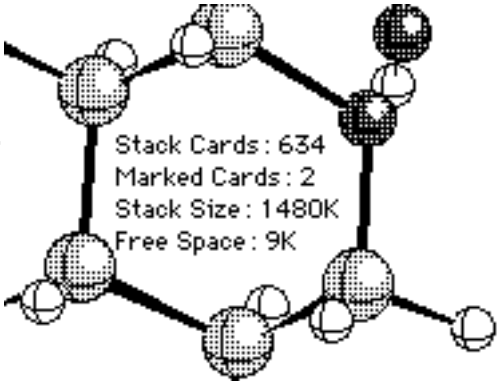
The Top Card

When you launch the NMR Database you see the following screen.



The Status Box

The status box, the text field below the stack name, tells you how many compound cards are currently in the stack, how many of them are marked, the amount of disk space used by the stack, and how much space could be reallocated if a Compact Stack operation (p. 5) was performed.



The Icons

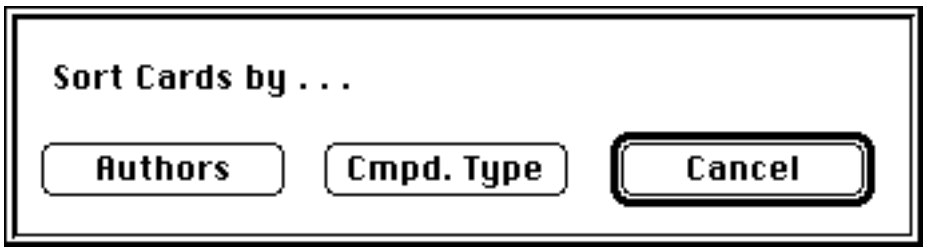
Many operations can be performed on the database from the top card. Each of the icons is described below.

Clicking on the view icon displays the cards in the stack sequentially starting with the first card. An option-click will display only the marked cards. Viewing can be stopped by pressing the mouse button.

If you pressed this icon and want to quickly get back to the NMR Database stack, press the ~ key or select Back from the Go menu.

Brings you to your HyperCard home stack. If you are not otherwise familiar with HyperCard, this may provide you with a jumping-off point to other applications.

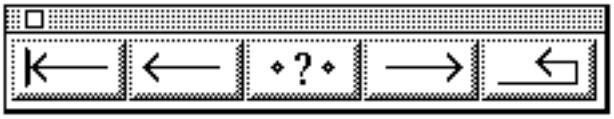
Clicking on the sort icon allows you to either alphabetically sort cards by authors or mark cards of a specified compound type. Compound Type sorting is more powerful than it looks from this simple dialog box (see p. **).



Clicking on the return arrow displays the most recently pushed card. An option-click brings up the most recently displayed card.

Displays a scrolling text field containing database version notes. It can be hidden by clicking again on the icon or by clicking in the notes field. This field is used mainly to keep track of minor changes to the database and to document features that may not be in the manual.

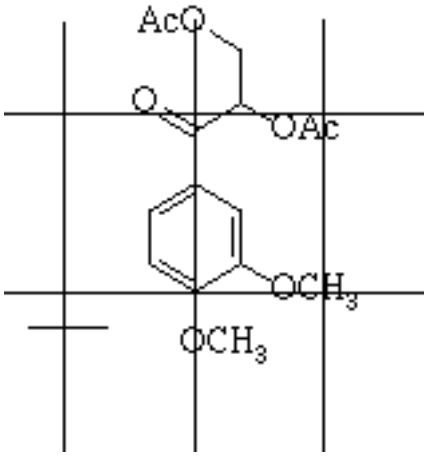
Clicking this icon displays the navigation palette. The symbols, in order, mean Go To First Card (Top Card), Go to Previous Card in the Database, Go To Any Selected Card Number,



Go To Next Database Card, and Return From Wherever You Came From (most useful if runing other Hypercard applications).

Brings up information about the authors of this Database. Clicking in the displayed fields causes them to go away.

The pack icon is used to free up unused space which accumulates after various operations. The amount of space which can be reclaimed is displayed in the status field on the Top Card.



This icon toggles the structure grid on and off. The grid can be useful when trying to position a new structure on the card.

This icon brings up a pop-up menu which allows you to jump directly to a specific bookmarked card in the stack. This menu can be modified by adding and removing bookmarks from cards.

The closed lock icon indicates that the data in the database is protected and cannot be changed. To open the lock click on the icon with the option key held down. When prompted for a password type *NMR*. Obviously this is not for high security — it is just to avoid accidental loss of data.

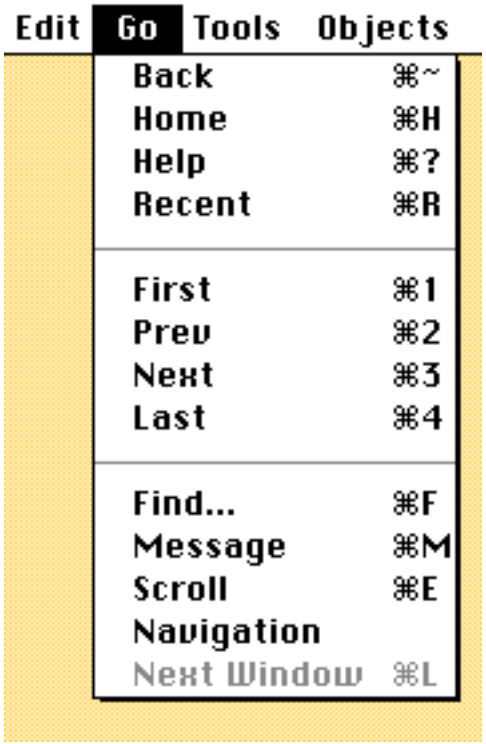
An open lock icon means that all of the data fields are editable and that new structure may be added to the database. To close the lock and protect the stack click on the lock icon.

The group one and two buttons are used to select which card groups will be included when doing searches that mark cards. Group one consists of compounds run in three solvents specifically for this database. Other compounds and literature data are in the group two section. Group two compounds are by default all cards starting at 10000.

Moving Around

There are three methods which can be used to move around in the NMR Database stack. The menus, the keyboard, and the navigation palette.

The Go Menu



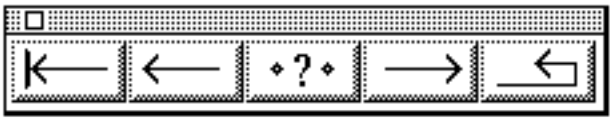
The Go Menu allows logical navigation and provides command-key equivalent for those familiar with Hypercard conventions. Recent brings up thumbnail views of the last cards visited — clicking on one will take you to that card.

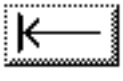
The Keyboard

The arrow keys on the Macintosh extended keyboard can be used to navigate within the stack. The left arrow key moves you to the previous compound card. The right arrow key moves you to the next card. If the option key is held down while pressing the right arrow key, the next *marked card* will be displayed. Likewise, if the left arrow key is pressed while holding the option key down, the previous *marked card* is brought up.

The Navigation Palette

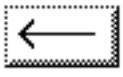
The navigation palette can be displayed by selecting “Navigation” under the Go menu or by clicking on the navigation button on the top card. The left and right arrow buttons on the navigation palette have the same function as the previous and next buttons on the keyboard.





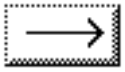
Displays the top card.

Option Key Enhancement

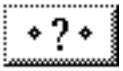


Displays the previous card. If the option key is held down while pressing the previous button, the previous *marked card* will be displayed.

Option Key Enhancement

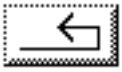


Displays the next card. If the option key is held down while pressing the next button, the next *marked card* will be displayed. Clicking the next button while pressing the shift key causes a ‘show all cards’ starting at the the current card. Clicking the next button while pressing the shift and option keys shows all marked cards starting at the current card.



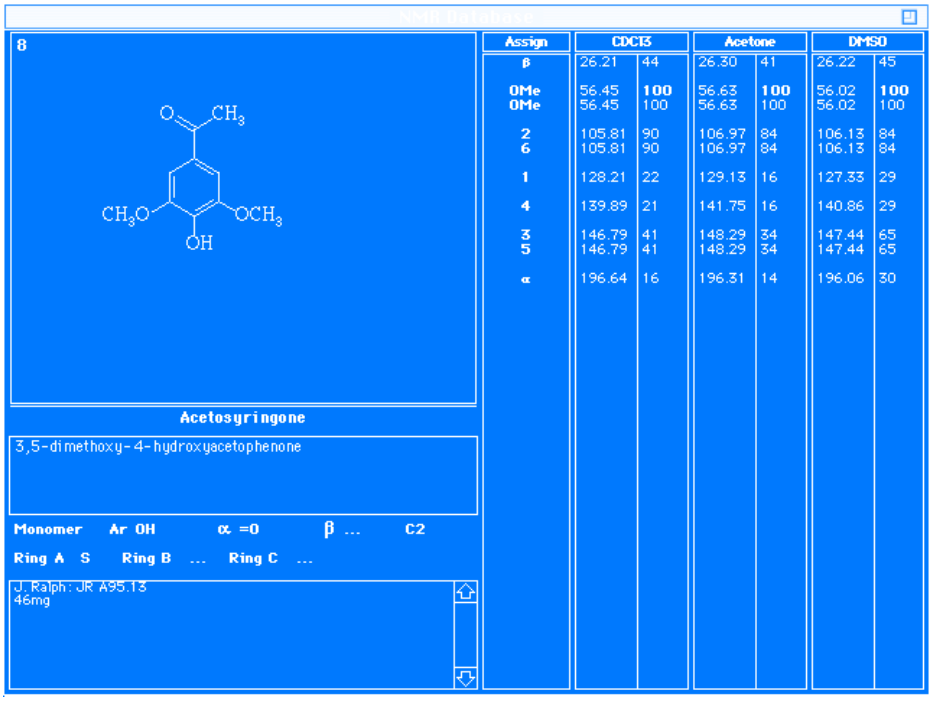
Allows you to go directly to a specified card number.

Clicking the “Go to Which Card?” button while pressing the option and shift keys either locks the database if it is currently unprotected or unlocks it if the database is protected. The password is required to unlock the database.



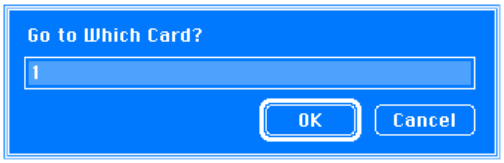
Returns you to the card you were at when you pressed the display top card button on the navigation palette.

Card Layout



Card Number

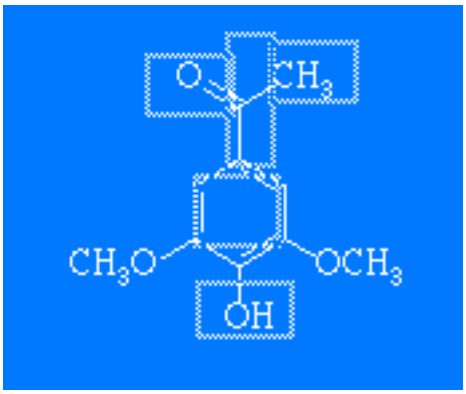
Clicking on the card number brings up the "go to which card" dialog box allowing you to go to a specified card.



Structure

Clicking on various portions of the structure initiates searches for similar structures.

In this figure, the locations of the transparent attribute buttons for a typical structure are indicated.



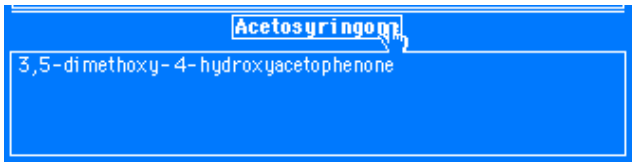
Marked Flag

The marked flag indicates that a card has been marked manually or as the result of a search.

Clicking on the word Marked will unmark the card. Clicking again will mark the card.

Compound Name

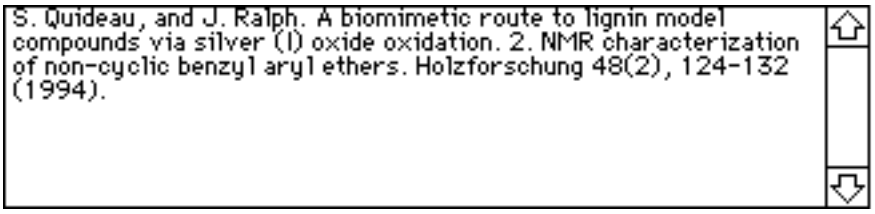
Clicking in one of the regions containing the compound name results in a search for an identical compound.



Each click brings up the next occurance of that compound name in the name field.

Reference Field

If the data for this compound has been published, the journal reference is the first line in the Notes field. If not, the lab book number and page or supplier is there.



The first line of the reference field is what is used to do the author sorting.

Shift Columns

Clicking in the assignment or shift headers of a card causes the data fields to display proton NMR data. Clicking again displays the original carbon NMR data.

H-Assign	H-Acetone	#H's	mult	J
β	3.61	1	br q	
A3OMe	3.82	3	s	
B3OMe	3.91	3	s	
γ	3.87-3.91	2	m	
α	5.65	1	d	6.60
β'	6.65	1	dd	15.8,7.7
A5	6.81	1	d	8.10
A6	6.88	1	dd	8.1,2.0
A2	7.04	1	d	2.0
B2	7.29	1	bro	
B6	7.32	1	bro	
α'	7.59	1	d	15.8
γ'	9.63	1	d	7.7

Assign	CDCl3		Acetone		DMSO	
A3 OMe	55.76	82	56.18	83	55.41	88
B3 OMe	55.85	92	56.20	83	55.61	**100**
C3 OMe	55.93	**100**	56.32	76	55.80	100
γ	62.17	40	61.75	46	59.74	31
Bγ	63.56	61	63.25	**100**	61.52	71
Cγ	63.63	64	63.25	100	61.58	72
α	81.68	52	81.15	49	79.01	39
β	85.42	56	85.31	57	82.53	40
C2	109.38	61	110.74	50	109.93	62
B2	109.54	56	110.93	51	109.93	62
A2	109.77	62	112.11	53	111.91	41

Searching for a Structure

The Find command is useful for finding an occurrence of a string of characters. It can be used to quickly find the next occurrence of a specific chemical shift, an author, a compound name, or any other piece of information that is displayed on a card.

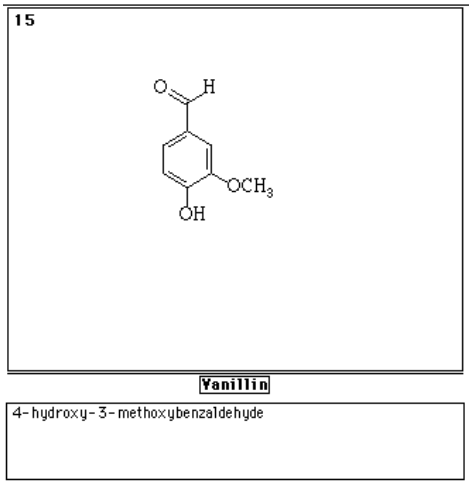
Using Find

To use the Find command, select “Find” under the Go menu. Type within quotes what you wish to find and press return.

The shortcut for Find is #F

The found selection will have a box drawn around it.

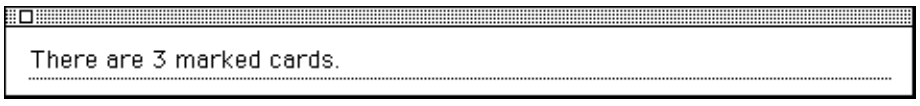
To repeat the search and find the next occurrence, press the return key again. This works only if the previous found selection is still boxed.



Marking Cards

A list of the currently marked cards can be viewed and printed by selecting List Marked Cards... under the Print menu.

Cards can be individually marked or unmarked by clicking in the region of the Marked Flag. The number of marked cards can be found by looking at the status field on the top card or by selecting *# Marked Cards* under the Edit menu.



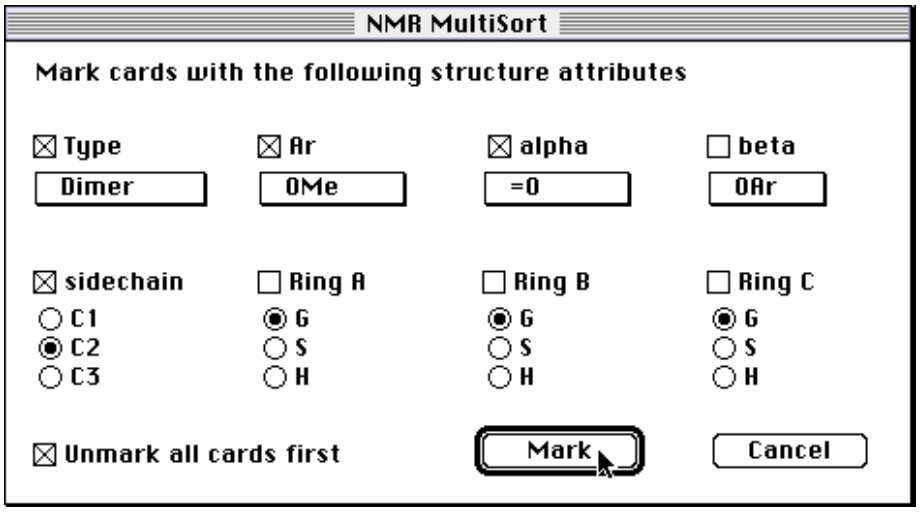
Shortcuts:
 # Marked Cards #J
Unmark all cards #U

All cards can be unmarked in one operation by selecting *Unmark All Cards* under the Edit menu.

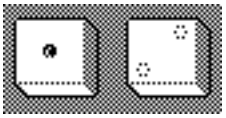
Using MultiSort

To search for a compound with specific attributes select By Compound... under the Search menu. This brings up a dialog box which enables rapid “multiple condition” marking of cards.

You can also get the MultiSort dialog box by selecting "By Compound" by using the sort icon on the top card.

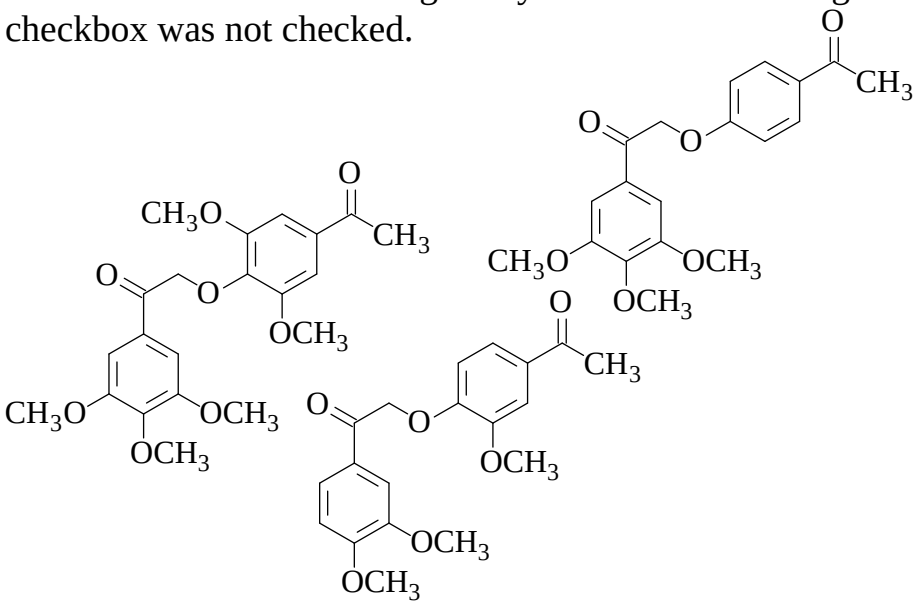


If only the group one icon on the top card was highlighted then any cards in group two that fit the specified description would have been ignored and not marked.



You define the compound to search for by clicking appropriate check boxes and selecting various properties from the pop-up menus. Each radio button and pop-up menu has a check box above it which activates the radio button or pop-up for searching. If the unmark all cards box is not selected, the compounds found matching your description will be added to the previously marked cards.

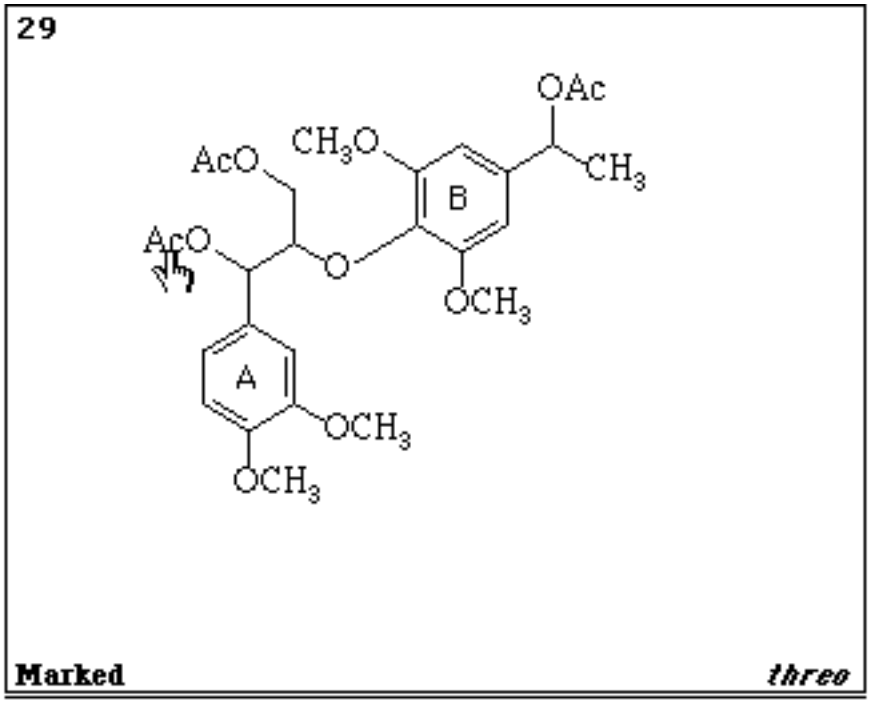
The attributes selected in the dialog box above describe all of the structures pictured here. Note that, for example, the search was not restricted to guaiacyl units since the Ring A checkbox was not checked.



Graphical Searching

Graphical structure sorting allows you to find structures which match in some way the one on the screen. Each structure has a set of transparent buttons which are used to indicate the part of the structure to sort by.

For example, clicking on the alpha position of a structure will cause the computer to look at the a field in the structure description section of the card. If the field had in it AcO, then all of the cards with AcO in the alpha position would be marked.

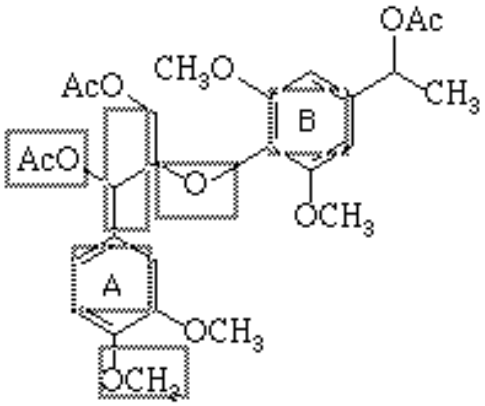


Yeratrylglycerol-β-syringol ether triacetate

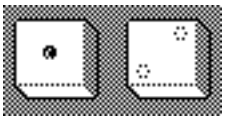
1,3-diacetoxy-1-(3,4-dimethoxyphenyl)-2-(4-(1-acetoxyethyl)-2,6-dimethoxyphenoxy)propane

Clicking on the A-Ring of a structure while holding down the shift key will result in a search based on compound size, (monomer, dimer, trimer, oligomer), not on ring type.

This Figure indicates typical positions for some of the structure buttons. Clicking in any one of these areas on a structure initiates a search on that part of the structure.



If only the group one icon on the top card was highlighted then any cards in group two that fit the specified description would have been ignored and not marked.



Before a graphical structure sort, first choose which card groups you wish to search.

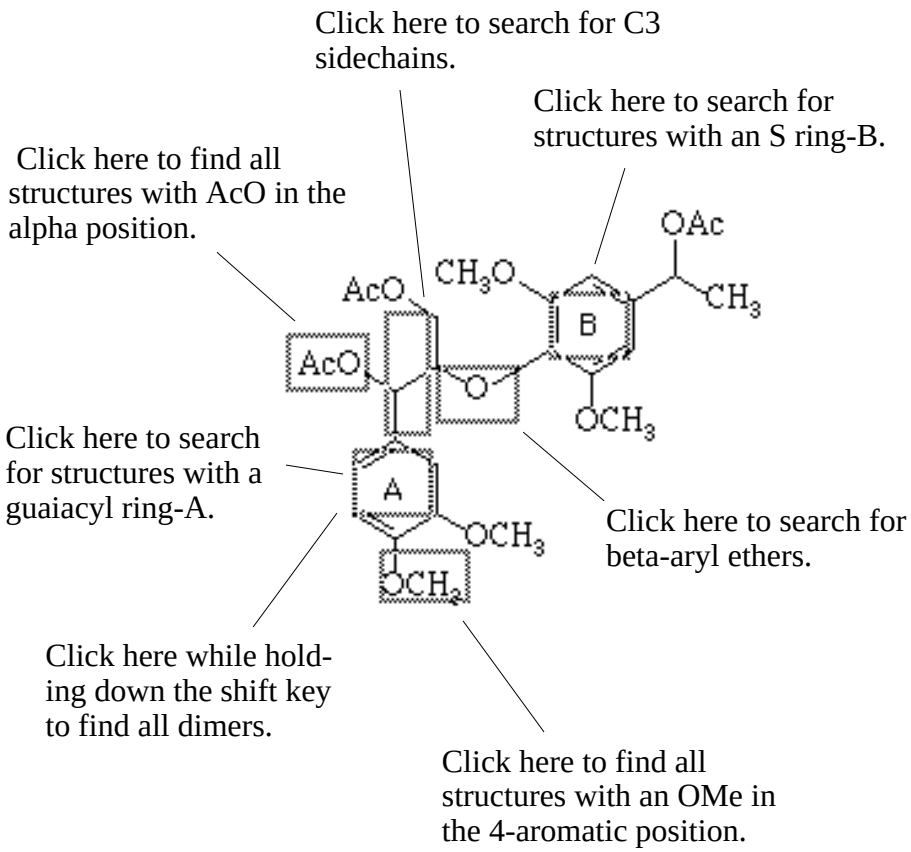
To begin a graphical sort click on the part of the structure that you wish to sort by. If there are no previously marked cards, all cards which match the part of the structure you clicked on will be marked.

If there had already been some marked cards, only those cards already marked would have been considered in the search. The result is a reduced set of marked cards.

Option Key Enhancement

If the option key is held down while clicking, all cards with the indicated feature will be marked regardless of any cards that were marked previously. The result is an increased number of marked cards.

Graphical structure sorts do not need to be limited to clicking on different portions of one structure. You can reduce or expand the set by clicking on any number of different structures. For example: you could click on the A-ring of one structure and then move to a second structure and click on its alpha position. The result would be a set of marked cards that have the same A-ring type as the first structure and the same alpha attribute as the second structure.



Searching for Shifts

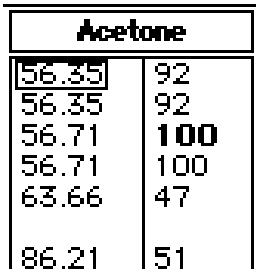
There are three methods provided for searching for compounds with specific shifts.

Using Find

The Find command can be used for finding a single occurrence of a specific shift. To use the Find command, select “Find” under the Go menu. Enter the shift between the quotes and press return.

The shortkut for Find is #F

The found selection will have a box drawn around it.



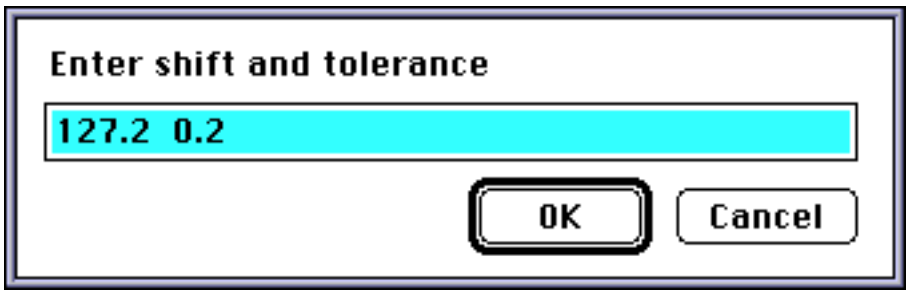
To search for the next occurrence of the shift press the return key again. This works only if the previous found selection is still boxed.

Using Shift Range Simple

To search for all of the occurrences of a shift select Shift Range Simple... under the Sort menu. The dialog box allows you to specify a shift and tolerance.

All cards are first automatically unmarked when this search is performed.

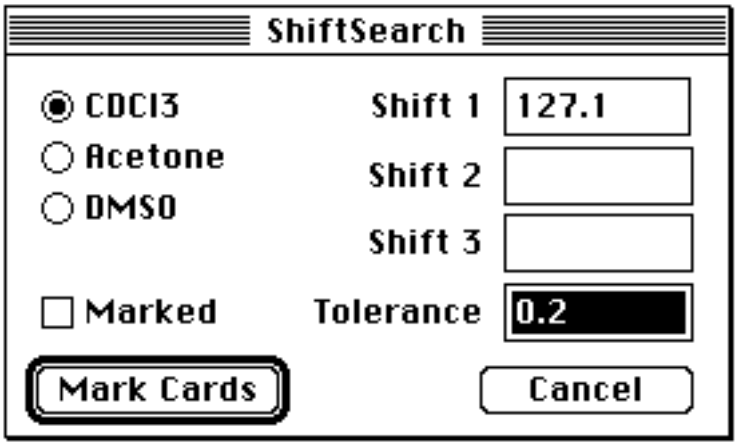
Also note that this operation will mark cards regardless of which group they are in and which group buttons are activated.



All cards containing a shift within the specified range will be marked.

Using Mark Shift Range

Selecting Mark Shift Range... under the Sort menu brings up a dialog box with more options than the Shift Range Simple... command.



The Mark Shift Range command does take into account which group buttons are activated ont he top card. Only cards in the selected groups will be searched.

Radio buttons allow you to limit the search to within a specific solvent. If more than one shift is entered, both or all three shifts must occur in a compound for it to be marked. The tolerance value creates a range of possible values for each shift entered.

Clicking in the Marked checkbox indicates that only marked cards will be considered in the search. If the Marked checkbox is not checked, all cards will be unmarked before the search begins.

Sorting Cards

Some of the operations in the Sort menu change the physical ordering of the cards in the database.

Sorting by Authors

You can also sort by authors by selecting "By Authors" using the sort icon on the top card.

This alphabetizes the cards with respect to the notes field.

Moving Marked Cards to Front

Marked To Front reorders the stack by grouping together and bringing all of the currently marked cards to the front of the stack. The top card of the stack will still remain at the front.

Moving Marked Cards to Rear

This moves all marked cards to the rear of the stack.

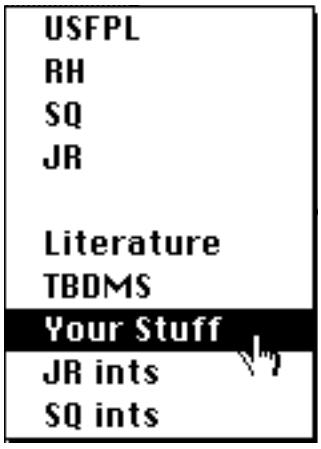
Unsorting Cards

Reorder returns the stack to its original sequence. If the Reorder menu item is disabled that means that the stack is all ready in its original sequence.

Setting Bookmarks

Bookmarks allow you to quickly jump from the top card to any one of the bookmarked cards in the database.

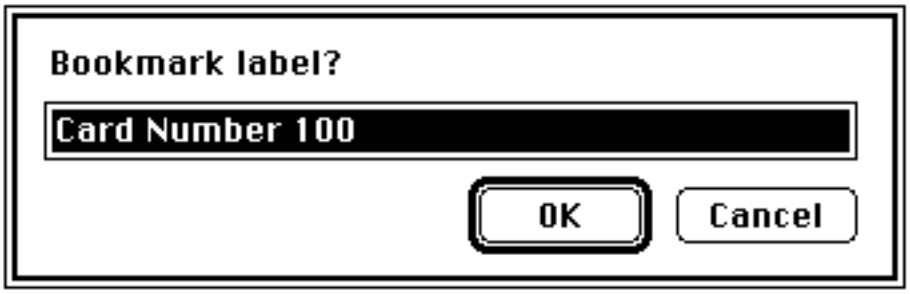
You jump to a bookmarked card by selecting it from the bookmark list pop-up menu on the top card.



The label "Your Stuff" is where your compounds should be placed if you want them to be distributed with the database.

If the "Add Bookmark..." menu item is disabled that means that the current card already has a bookmark on it.

A bookmark can be attached to a compound card by selecting “Add Bookmark...” from under the Edit menu and giving it a label. The bookmark label is what shows up in the bookmark list pop-up menu on the top card.



To change the label of abookmark first remove the current bookmark and then add a new one.

Once a bookmark has been added it will show up in the bookmark list pop-up menu on the top card.

A bookmark can be removed by going to the bookmarked card and selecting “Remove Bookmark” from under the Edit menu.

Printing Cards

The print menu enables you to print a single card, all of the cards, all of the marked cards, a range of cards, or a range of marked cards.

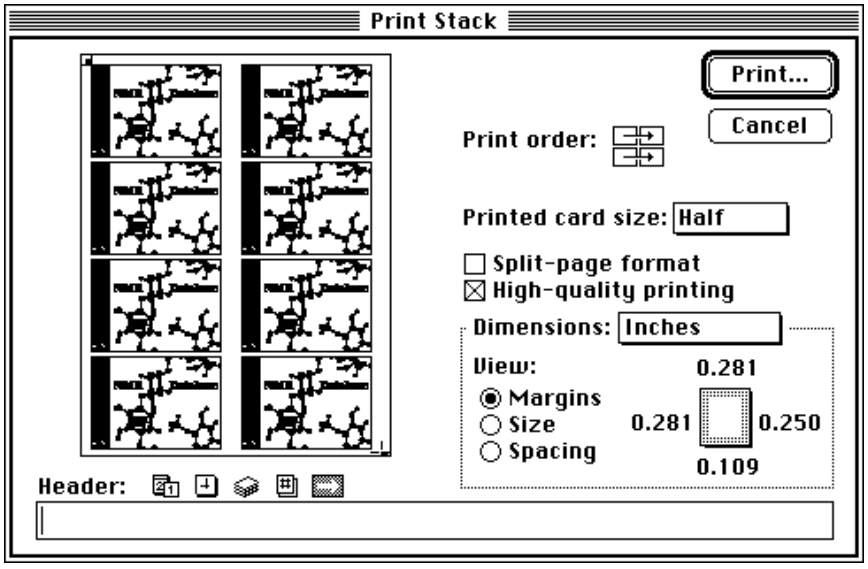
One Card

This prints the card currently displayed on the screen to the selected printer.

All Cards

Print All... Prints all of the cards in the stack.

This dialog box comes up after selecting one of the Printing menu items. It is a standard Hypercard dialog box described in your manuals.



Marked Cards

Print All Marked... Prints all of the marked cards in the stack.

Range of Cards

Print Range allows you to print all of the cards between two locations in the stack. The first card to print is set by going to the desired card and clicking on the starting card requester.

You may set the last card to print before setting the first one by dragging the starting card requester off of the last card requester. Also, the operation may be canceled by clicking in the close box of each requester.

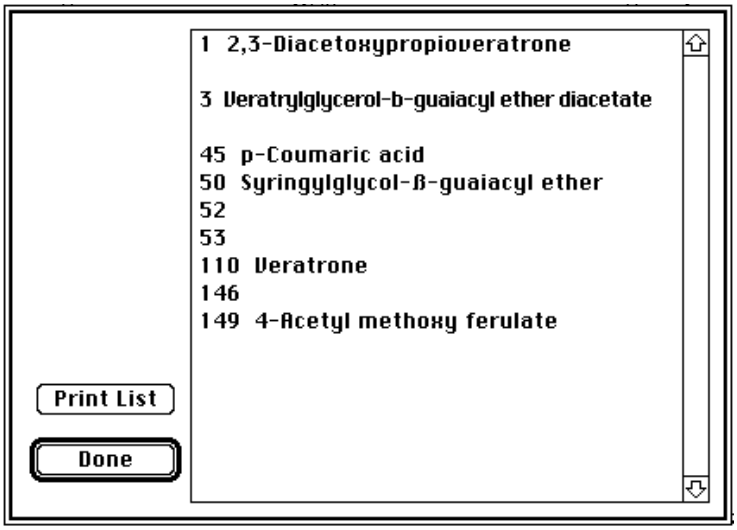
The last card to print is set the same way.

Range of Marked Cards

Print Range - Marked Cards is identical to “Print Range...” with the exception that it will print only the marked cards between the two endpoints that you indicate. Unless they are also marked, the set of cards printed will not include the two endpoints.

Listing Marked Cards

The last item under the Print menu is List Marked Cards... This allows you to view and print out a list of the currently marked cards.

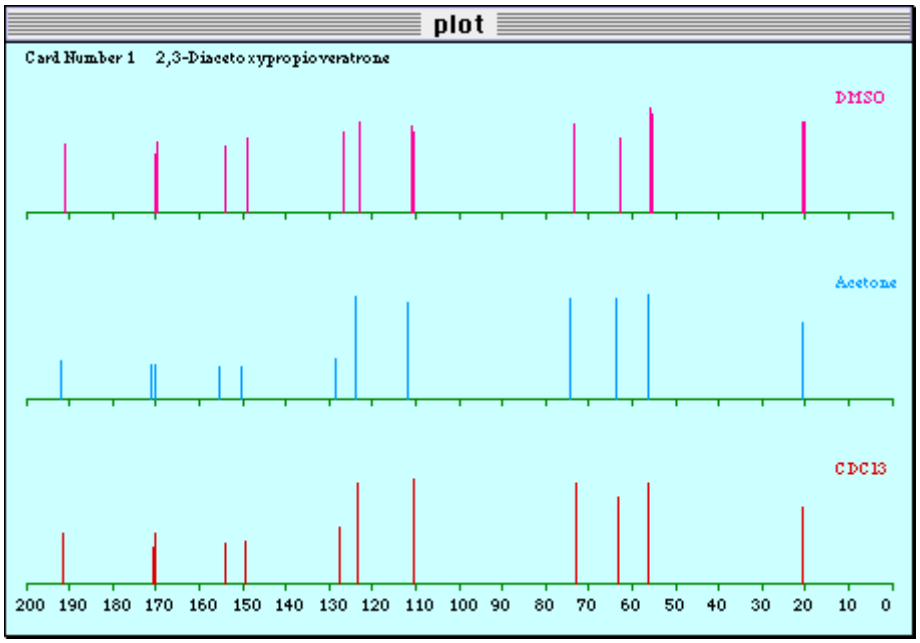


Viewing Spectra

The Spectra menu allows you to view a plot of the spectra of the data on the current card. If the intensity data is recorded on the cards, the appearance of the spectra will be as run (except for the absence of noise).

Selecting Plot Spectra under the Spectra menu displays a plot of the current card's shift and intensity data.

*If the intensities on the data card have not yet been normalized (as a percentage of the tallest peak), this graphing operation will normalize the intensities first. If a data set has been normalized, a bold **100** appears in each intensity column.*

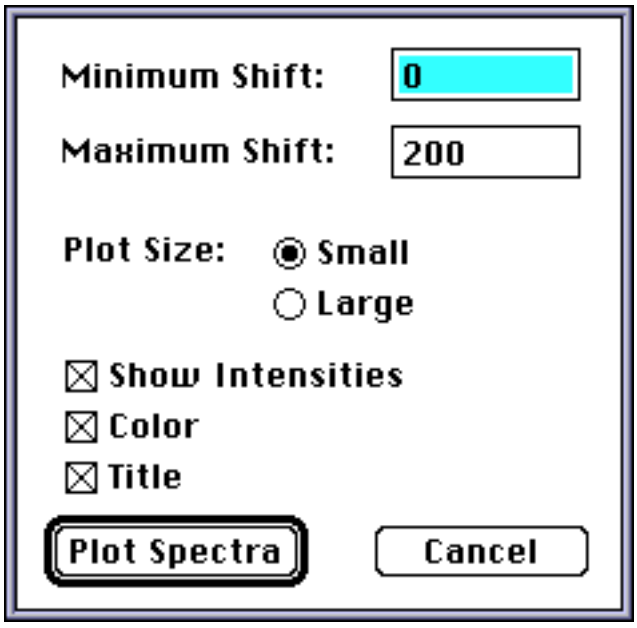


Select Close Plot from under the Spectra menu to close the plot.

Setting Options

The plot format can be customized by selecting Set Options from under the Spectra menu.

The options selected in this dialog box become the default options used to plot spectra.



To enlarge a portion of the plot where shifts are close together, change the Minimum and Maximum shifts so only the portion you are interested in is plotted.

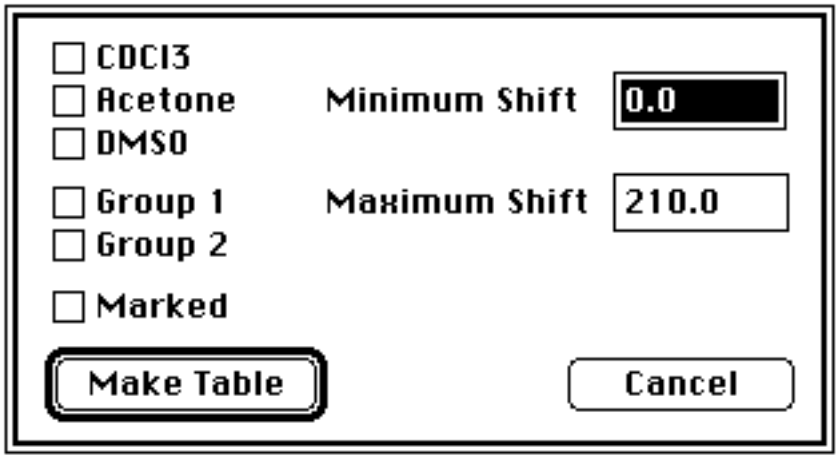
The large plot size option is useful when the plot will be used in a graphics program. The larger plot size saves more data and produces higher resolution in graphics programs.

Saving the Plot

The plot can be copied to the clipboard as a PICT using Clip Plot from under the Spectra menu. The plot can also be saved in PICT and HPGL formats.

Making a Shift Table

A hardcopy listing of the chemical shifts in the database can be created by selecting "Make ShiftTable" from under the File menu. A dialog box is displayed which enables you to choose which shifts will appear in the table.



There is no way to tell which solvent produced a specific shift by looking at the shift table only.

The three clickboxes labeled CDCl3, Acetone, and DMSO determine which solvent field on each card will be included in the table.

The group icons on the top card are ignored when making a shift

The clickboxes labeled Group 1 and Group 2 indicate which of the two groups of cards will be included in constructing the table.

If you want only the marked cards to be put into the table then check the clickbox labeled Marked. This works with any combination of the other clickboxes activated. For example, you could choose to have only shifts from structures in group 1 that were marked and run in acetone.

The range of shifts to be put into the table is set by entering the minimum and maximum shifts desired in the respective fields. Defaults are set which give the entire range of normal shifts.

A typical line of the output will be a chemical shift followed by a list of the cards which contain that shift. The chemical shifts, within the range specified, are listed in 0.1 increments. The output is a simple text file which can be opened and reformatted in a word processor. The raw text file for a shiftTable of all shifts will consist of close to 100 pages of data so formatting is desirable as the output can easily be reduced to better than 50%.

A sample of the formatted shift table for shifts as specified in the above dialog box is shown below.

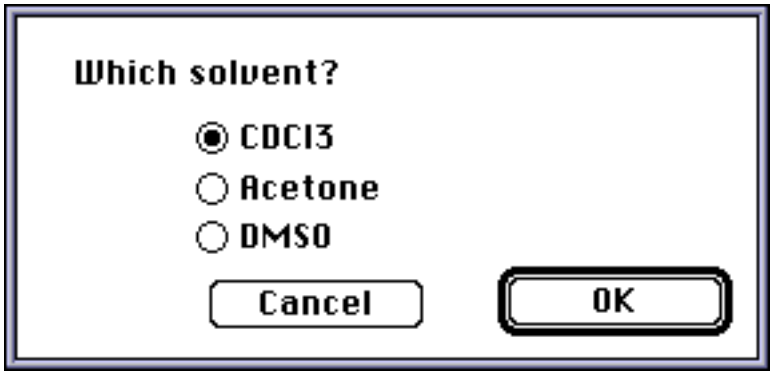
stack “NMR Database” 10/20/93 2:40 PM
Solvents included: CDCl3
Group 1
Minimum Shift: 55.0
Maximum Shift: 57.0

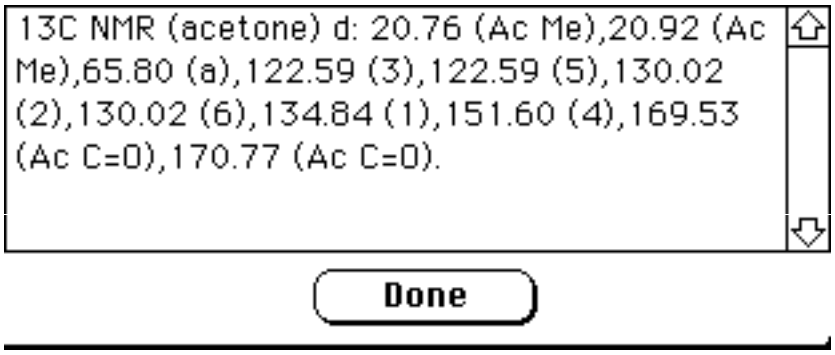
55.0:
55.1:
55.2: 37 2019
55.3: 25 59
55.4: 20 36
55.5: 2006
55.6: 86
55.7: 3 5 78 85 92 99 111 162 2001 2005 2015 2016 2022 2024
55.8: 2 3 11 13 27 29 31 39 50 56 70 74 75 76 77 82 83 84 87 88 90 97 101 104...
55.9: 5 9 13 19 21 29 32 33 34 35 47 66 67 68 69 70 73 74 75 76 77 78 81 82 83..
56.0: 1 2 7 9 15 22 26 29 44 52 55 57 65 71 73 84 98 103 106 116 120 133 139...
56.1: 1 57 62 63 89 110 134 135 146 154 161 2008 2018 2019 3004 3007
56.2: 12 16 40 79 92 97 98 99 100 114 123 155 161 2002 3004 3007
56.3: 26 27 50 52 53 60 79 80 81 88 89 90 91 121 156 1004 3004 3007
56.4: 8 21 22 41 51 64 117 153
56.5: 130
56.6:
56.7:
56.8:
56.9:
57.0:

Experimental Data

You can even use the database to write parts of your experimental section for you (if you put your own data in here).

The Exptl-C... and Exptl-H... menu options under the File menu allow you to create a text file for the data on the card. You can then copy and paste this to your word processor. Only a few fonts (the greek letters) and super/subscripts will need changing. The format is ACS format.





Holding down the option key while clicking the Done button will copy the data to the clipboard to save you from having to select the text and copy it from the Edit Menu.

Option Key Enhancement

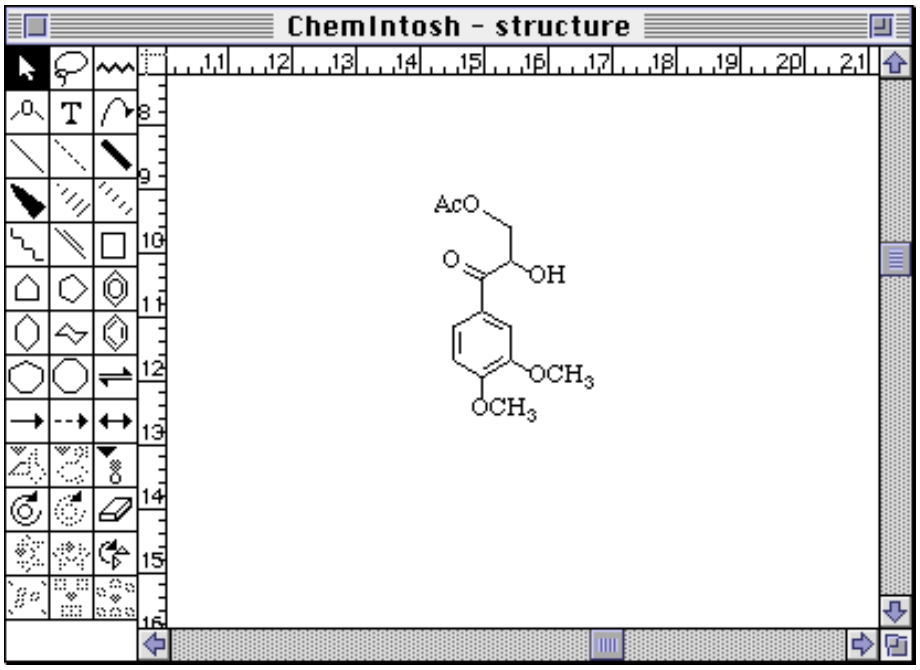
Simple formatting in your word processor will make the data look something like this . . .

^{13}C NMR (acetone-d_6) δ: 20.76 (Ac Me), 20.92 (Ac Me), 65.80 (α), 122.59 (3), 122.59 (5), 130.02 (2), 130.02 (6), 134.84 (1), 151.60 (4), 169.53 (Ac C=O), 170.77 (Ac C=O). ^{1}H NMR ($CDCl_3$) δ: 1.45 (3H, d, J = 6.4, B β), 3.85 (3H, s, OMe), 3.85 (3H, s, OMe), 3.87 (3H, s, OMe), 3.89 (2H, s, OMe), 4.81 (1H, q, J = 6.4, B α), 5.02 (1H, d, J = 8.7, α), 6.63 (2H, s, B2/6), 6.9 (H, J = 1.8, A2), 6.83 (1H, d, J = 8.7, A5), 6.9 (H, J = , A6).

Editing Structures

Many of the structures in the database have SCF files asscociated with them so that users of Chemintosh 3 (Softshell International) will be able to edit them.

To edit a structure select "Edit Structure" from under the Edit menu. If Chemintosh 3 is located on your system, a file will be opened showing the structure.



Not all structures in the current Database release have associated SCF files at present.

Exporting Data

There are three different methods for exporting data from the NMR Database. All three export functions are under the File menu.

Export Your Stuff..

This menu item exports all of the compounds that you have entered in the location bookmarked as "Your Stuff" into a text file that we can use to integrate your compounds permanently into the database.

Export...

This allows you to export data from any compound card into a text file. All data is exported in a tab seperated column format. If the Data Only check box is selected, there will be no descriptive headers above the data columns in the exported file.

FileMaker Export...

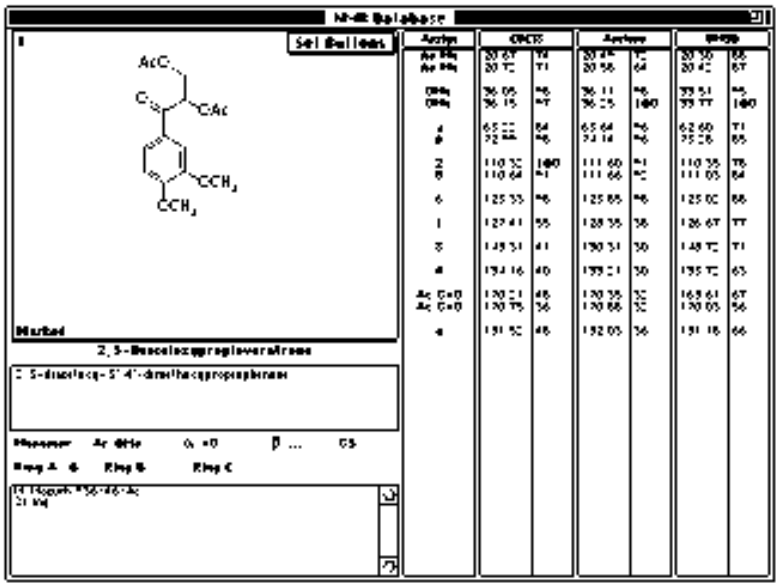
This export command exports data in a format compatable with FileMaker Pro.

Adding Compounds

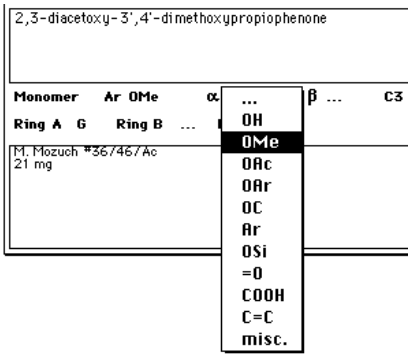
Holding down the shift and option keys while clicking on the “Go to which card” palette button will unlock the stack given the proper password. The same thing can be done to lock the stack.

During normal use the database is protected from accidental data changes by always leaving it locked. In order to make changes or to add new compounds the database must be unlocked. To unlock the database, hold down the option key and click on the closed lock icon on the top card. A requester will appear and ask for the password. Type in “nmr” and press return. The fields on each card are now unlocked and editable. Clicking on the open lock icon on the top card will close the lock and protect the database. Quiting the database will also cause the lock to close.

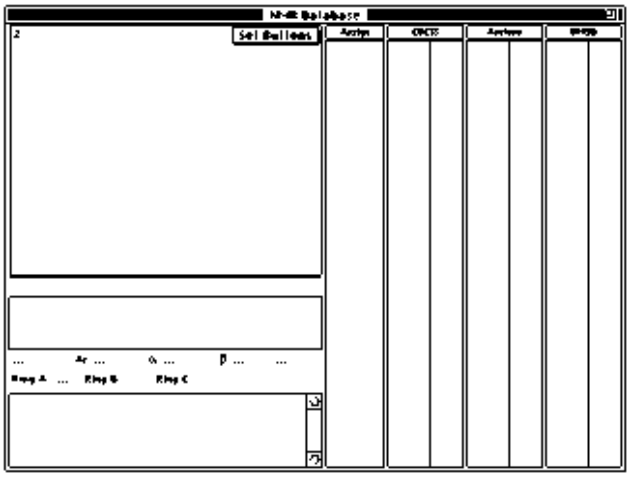
When the stack is unlocked all of the text fields become editable and many hidden buttons become active. The only obvious change is the presence of a new button, "Set Buttons".



Another change is that all of the compound attributes become pull down menus.



To add a new card after the currently displayed card select “New Card” from the Edit menu.



It is recommended that you place your new cards in the "Your Stuff" section.

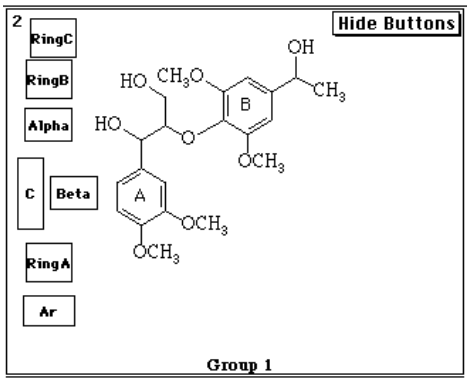
Note that the card number in the top left corner of the structure box is simply the number on the previous card incremented by one. This can be changed by clicking on the card number while holding down the option key and entering a new number in the requester. Text fields may now be filled by clicking on a field and entering the appropriate data To enter proton data click on one of the headers to bring up the proton data fields. Intensity data will be automatically normalized with 100 as the largest peak after the first time the data is plotted using Plot Spectra under the Spectra menu. Note that when the data has been normalized the 100 in the intensity column is shown in bold.

Original intensity data can not be retrieved once it has been normalized so check the non-normalized data carefuly before plotting the data.

Assign	CDCl3	
B β	25.45	34
OMe	55.87	**100**
OMe	55.87	100
B OMe	56.08	99
B OMe	56.08	99
γ	60.48	29
B α	70.11	43
α	73.98	39
β	88.94	37
B2	102.25	67
B6	102.25	67

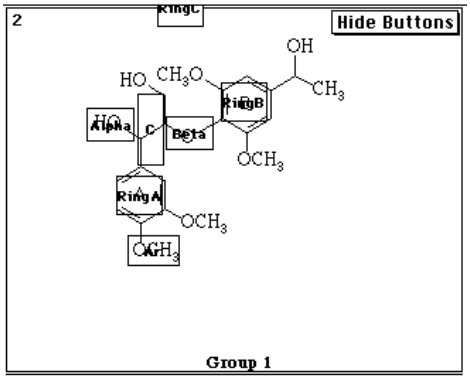
The structure can be pasted onto the card as a bitmap and then positioned in the structure box. Depending on the drawing program used, you may need to select the transparent feature under the Paint menu of HyperCard after pasting the bitmap.

The structure buttons which make the graphical searching possible are transparent buttons placed over certain portions of the structures. For the searches to work correctly, the buttons must be placed in the appropriate locations. To position the buttons, press the button in the upper right corner of the structure box labeled “Set Buttons”. This will make the structure buttons appear as rectangles with labels and allow you to drag them into position.



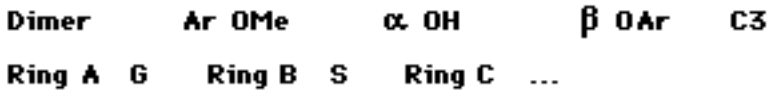
For examples of where to place the buttons, you can press the option and command keys simultaneously to see where the buttons were placed on different kinds of structures. This also works when the stack is locked.

Drag the RingA button over the A-Ring of the structure, the Alpha button over the alpha position of the structure, and the remaining buttons over their associated structure positions if they exist. If your structure has no C-Ring then simply leave it to the side of the structure box or drag it to the edge until only a portion of it is visible.



The group type should also be selected at this time. Click in the bottom middle portion of the structure box to select the correct group type. Group 1 compounds are typically reserved for compounds done at our labs while Group 2 type compounds are all others. When finished press the button in the corner which is now labeled “Hide Buttons”.

A structure button works by initiating a search on the string which occurs in its associated compound description field. For example, if the a field of a card contains an OH then clicking on the alpha position of the card's structure will result in all cards whose a field contains an OH to be marked.



The first row of structure description fields are pull down menus. The correct attributes for a new structure should be selected after pasting the structure on a new card. The three ring type fields are filled by clicking on the field repetitively until the proper ring type, (either G, S, or H), is displayed.

If you have created a few new cards, set the button positions on the first card and then go to the next one. It is not necessary to click “Show Buttons” and “Hide Buttons” for each card. This is useful if you have many cards and want to check the button positions. Simply start at the beginning and press “Show Buttons”. Now view each card checking the buttons, repositioning them when necessary.

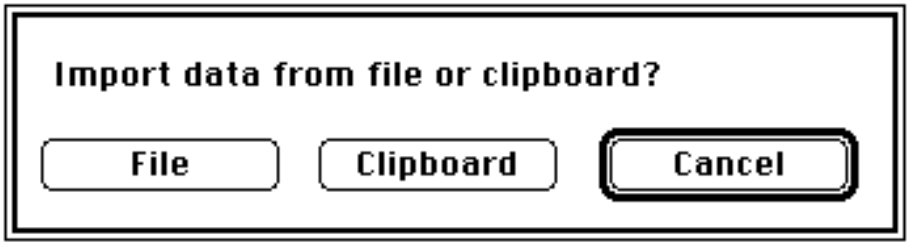
The isomer field is a pop-up menu in the lower right corner of the structure box which should be selected accordingly.

The first line in the notes field should contain a journal reference if one exists or an identifier like the lab book number.

Importing WinNMR Data

Adding data to the cards by hand, particularly with intensity data is a pain. For those who have Bruker's Win-NMR program, this Database offers a simple import method.

From Win-NMR, create a Peak Picking report. Select the data and copy it to the clipboard or save it as a text file. In the Database, select "Import Win-NMR Data" from the File Menu.



Then simply answer the following dialog box pertaining to solvents to put all shift and intensity data into the appropriate columns. Depending on the quality of the peak picking, you may still need to edit to some extent (e.g. remove solvent peaks).